

10/751,388

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:47:02 ON 13 JUL 2007

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:47:13 ON 13 JUL 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 JUL 2007 HIGHEST RN 942260-92-6

DICTIONARY FILE UPDATES: 12 JUL 2007 HIGHEST RN 942260-92-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

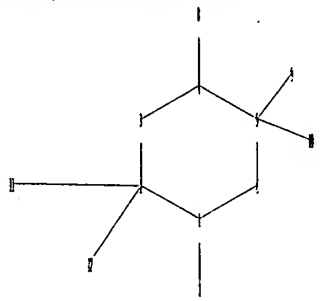
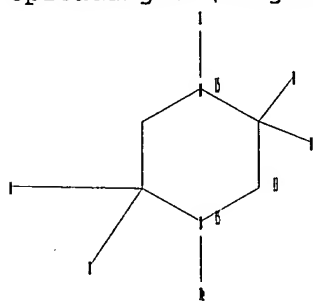
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10751388.str



chain nodes :

7 8 9 10 11 12

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 2-11 2-12 4-8 5-9 5-10

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

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1-2 1-6 2-3 3-4 4-5 5-6
exact bonds :
1-7 2-11 2-12 4-8 5-9 5-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 10:47:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 69561 TO ITERATE

2.9% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1375516 TO 1406924
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> scr 2039

L3 SCREEN CREATED

=> s l1 and l3

SAMPLE SEARCH INITIATED 10:48:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 192 TO ITERATE

100.0% PROCESSED 192 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3009 TO 4671
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L1 AND L3

=> s l1 and l3 full

FULL SEARCH INITIATED 10:48:58 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3784 TO ITERATE

100.0% PROCESSED 3784 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L5 4 SEA SSS FUL L1 AND L3

=> d l5 1-4

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L5 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2007 ACS on STN
RN 877154-66-0 REGISTRY
ED Entered STN: 17 Mar 2006
CN Piperazine, 1-methyl-, labeled with deuterium (9CI) (CA INDEX NAME)
MF C5 H8 D4 N2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
IL 4H-2



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2007 ACS on STN
RN 791743-80-1 REGISTRY
ED Entered STN: 02 Dec 2004
CN Piperazine, 1-methyl-, labeled with carbon-13 (9CI) (CA INDEX NAME)
MF C5 H12 N2
CI COM
SR CA
IL XC-13



L5 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2007 ACS on STN
RN 119550-27-5 REGISTRY
ED Entered STN: 10 Mar 1989
CN Piperazine, 1-methyl-, labeled with tritium (9CI) (CA INDEX NAME)
MF C5 H12 N2
SR CA
LC STN Files: CA, CAPLUS, CASREACT
IL XH-3



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2007 ACS on STN
RN 112023-61-7 REGISTRY
ED Entered STN: 25 Dec 1987
CN Piperazine, 1-methyl-, labeled with carbon-13, dihydrochloride (9CI) (CA INDEX NAME)
MF C5 H12 N2 . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
IL XC-13
CRN (791743-80-1)



●2 HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

181.70

181.91

FILE 'CAPLUS' ENTERED AT 10:50:00 ON 13 JUL 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 13 Jul 2007 VOL 147 ISS 4

FILE LAST UPDATED: 12 Jul 2007 (20070712/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> d his

(FILE 'HOME' ENTERED AT 10:47:02 ON 13 JUL 2007)

FILE 'REGISTRY' ENTERED AT 10:47:13 ON 13 JUL 2007

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 SCR 2039

L4 0 S L1 AND L3

L5 4 S L1 AND L3 FULL

FILE 'CAPLUS' ENTERED AT 10:50:00 ON 13 JUL 2007

=> s 15

L6 3 L5

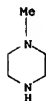
=> d ibib abs hitstr 1-3

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:619662 CAPLUS
 DOCUMENT NUMBER: 144:254085
 TITLE: Syntheses of [14C] and [2H4]PD0205520, an inhibitor of the tyrosine kinase activity of the epidermal growth factor receptor
 AUTHOR(S): Zhang, Yinsheng; Huang, Yun; Huang, Che C.
 CORPORATE SOURCE: Radiochemistry Group, Chemical R&D, Michigan Pharmaceutical Sciences, Pfizer Inc., Kalamazoo, MI, 49007, USA
 SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2005), 48(7), 485-496
 CODEN: JLCRD4; ISSN: 0362-4803
 PUBLISHER: John Wiley & Sons Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:254085
 AB 5-(4-Methyl-piperazin-1-yl)pent-2-ynoic acid 4-[(3-chloro-4-fluorophenyl)amino]pyrido[3,4-d]pyrimidin-6-ylamide, PD0205520, was under investigation as a potential inhibitor of the tyrosine kinase (TK) activity of the epidermal growth factor receptor (EGFR) for cancer treatment. Both radio- and stable-isotope-labeled compds. were required for drug absorption, distribution, metabolism and excretion (ADME) and quant. mass spectrometry bio-anal. studies. PD0205520 14C-labeled in the pyrimidine ring system was prepared in seven steps in an overall radiochem. yield of 26% from [14C]thiourea. PD0205520 2H-labeled in the piperazine ring was synthesized in four steps in a 32% overall yield.
 IT 877154-66-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of carbon-14- and deuterium-labeled PD0205520)
 RN 877154-66-0 CAPLUS
 CN Piperazine, 1-methyl-, labeled with deuterium (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1989:135210 CAPLUS
 DOCUMENT NUMBER: 110:135210
 TITLE: Synthesis of [3H]clozapine
 AUTHOR(S): De Paulis, Tomas; Davis, Daniel A.; Smith, Howard E.; Malarek, David H.; Lieberman, Arnold A.
 CORPORATE SOURCE: Dep. Chem., Vanderbilt Univ., Nashville, TN, 37235, USA
 SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1988), 25(9), 1027-33
 CODEN: JLCRD4; ISSN: 0362-4803
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 110:135210
 AB [3H]clozapine was prepared with a specific activity of 9.9 Ci/mmol by reaction of 8-chloro-11-(methylthio)-5H-dibenzo[b,e][1,4]diazepine with an excess of [3H]N-methylpiperazine. The latter was prepared from N-methylpyrazinium bromide in ethanolic HCl by reduction at room temperature with tritium over 5% Rh on Al2O3.
 IT 119550-27-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and condensation reaction of, with dibenzodiazepine derivative, labeled clozapine from)
 RN 119550-27-5 CAPLUS
 CN Piperazine, 1-methyl-, labeled with tritium (9CI) (CA INDEX NAME)



L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1987:597467 CAPLUS
 DOCUMENT NUMBER: 107:197467
 TITLE: Chemistry of nitrogen mustard [2-chloro-N-(2-chloroethyl)-N-methylethanamine] studied by nuclear magnetic resonance spectroscopy
 AUTHOR(S): Golding, Bernard T.; Keibell, Michael J.; Lockhart, Ian M.
 CORPORATE SOURCE: Dep. Chem., University of Warwick, Coventry, CV4 7AL, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1987), (6), 705-13
 CODEN: JCPKBH; ISSN: 0300-9580
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 107:197467
 AB MeN(CH2CH2X)2 (I; X = Cl) (II) was converted into the N-(2-chloroethyl)-N-methylaziridinium ion (III), which was characterized by NMR. Reactions of II with strong nucleophiles (e.g., S2O32-) gave disubstitution products (e.g., I; X = S2O3-). The intermediacy of III was inferred from the 13C distribution in product from 13C-labeled II. Less reactive nucleophiles (e.g., thiourea) yielded disubstitution products via spectroscopically detected intermediates III and ClCH2CH2NMeCH2CH2X (IV; e.g., X = SC+(NH2)2). Weaker nucleophiles (e.g., guanosine) did not give substitution products. Reaction of II with NH3 gave a 3-2 ratio of I (X = NH2) and N-methylpiperazine (V). I (X = NH2) was formed from III, while V arose from intramol. cyclocondensation of IV (X = NH2).
 IT 112023-61-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 112023-61-7 CAPLUS
 CN Piperazine, 1-methyl-, labeled with carbon-13, dihydrochloride (9CI) (CA INDEX NAME)



●2 HC1

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=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	16.75	198.66
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.34	-2.34

STN INTERNATIONAL LOGOFF AT 10:51:16 ON 13 JUL 2007